

# Numerical simulation of a polymer melting process using solar energy

J. Núñez<sup>a,\*</sup>, A. Beltrán<sup>b</sup>, M. Rivero<sup>b</sup> and J. Vega<sup>c</sup>

<sup>a</sup> *Escuela Nacional de Estudios Superiores, Unidad Morelia, UNAM,*

*Antigua Carretera a Pátzcuaro No. 8701, Col. Ex Hacienda de San José de la Huerta, Morelia, 58190, Michoacán, México.*

*\* e-mail: joseng@enesmorelia.unam.mx*

<sup>b</sup> *Instituto de Investigaciones en Materiales, Unidad Morelia, UNAM,*

*Antigua Carretera a Pátzcuaro No. 8701, Col. Ex Hacienda de San José de la Huerta, Morelia, 58190, Michoacán, México.*

<sup>c</sup> *Universidad de la Ciénega del Estado de Michoacán de Ocampo, Sahuayo, Michoacán.*

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In this work, the melting process of a polymeric material is numerically investigated. In general, the heat required for melting plastics is obtained throughout electrical resistances or by burning fossil fuels. The heat transfer mechanisms of these common practices correspond to conduction and convection, respectively. This work explores the feasibility of using radiation as the primary mechanism of energy supply, which has not been widely studied. The energy to achieve the phase change from solid to liquid can be obtained by concentrated solar energy radiation. The total energy required is calculated solving the energy equation using the enthalpy formulation. An explicit formulation with an enthalpy linearization was implemented in the Mathematica programming language and compared with the solution in the commercial software Ansys Fluent and COMSOL Multiphysics showing a good agreement. Based upon numerical predictions, it is examined the effects of the relevant parameters, such as incident radiation and convective heat transfer coefficient, on the melting process. It is observed that under weather conditions commonly attained in different cities worldwide, with a radiation of  $1000 \text{ W/m}^2$  and low convective losses with  $h = 8 \text{ W/m}^2 \cdot \text{K}$ , the melting process of a cylindrical rod of  $3/4$  inches diameter can be carried out in around 2 hours.

*Keywords:* Phase change; enthalpy formulation; radiation; heat losses.

En el presente trabajo, se investiga numéricamente el proceso de fusión de un material polimérico. En general, el calor requerido para fundir plásticos se obtiene a través de resistencias eléctricas o mediante quema de combustibles fósiles. Los mecanismos de transferencia de calor de estas prácticas comunes corresponden a conducción y convección, respectivamente. Este trabajo explora la factibilidad de utilizar la radiación solar como mecanismo principal de transferencia de calor, el cual no ha sido ampliamente estudiado. La energía para lograr el cambio de fase de sólido a líquido se puede obtener con radiación de energía solar concentrada. La energía total requerida se calcula resolviendo la ecuación de energía utilizando la formulación de entalpía. Se implementó una formulación explícita con una linealización de la entalpía en el lenguaje de programación Mathematica y se comparó con la solución en los softwares comerciales Ansys Fluent y COMSOL Multiphysics mostrando un buen ajuste. Con base en las predicciones numéricas, se examinan los efectos de los parámetros relevantes, como la radiación incidente y el coeficiente de transferencia de calor por convección, en el proceso de fusión. Los resultados muestran que bajo condiciones climáticas comúnmente encontradas en diferentes lugares del mundo, una irradiancia de  $1000 \text{ W/m}^2$  y bajas pérdidas por convección con  $h = 8 \text{ W/m}^2 \cdot \text{K}$ , se puede llevar a cabo el proceso de fusión de una barra cilíndrica con  $3/4$  de diámetro en alrededor de 2 horas.

*Descriptores:* Cambio de fase; formulación de entalpía; radiación solar; pérdidas de calor.

PACS: 01.50.My, Wg; 02.30.Hq; 01.55.+b; 06.30.Gv; 45.20.Jj; 45.20.dc; 45.40.Cc; 88.05.-b

## 1. Introduction

The melting process of materials is the phase change from solid to liquid. It is a very important phenomenon in several engineering applications, such as thermal energy storage, casting and moulding, crystal growth, welding, etc.

Several researchers have investigated the phase change process from the theoretical, numerical and experimental point of view. Analytical solutions of this type of phenomenon are very limited because they refer to a multi-phase and moving boundary problem, so they have been obtained essentially for very simple geometrical models, material types and conditions [1,2]. Important studies were specially focused on the numerical techniques for solving solidification and melting phase change problems [3]. Numerical methods dealing with phase change problems may be classified as in three categories: front tracking methods, fixed grid techniques and Eulerian-Lagrangian approach. Front tracking methods consider the solid-liquid interface as a boundary

between two domains (solid and liquid) where distinct sets of conservation equations are solved. An additional boundary condition is specified at the interface to account for heat transfer between the two domains. These methods require a moving adaptive grid that changes as time proceeds to reproduce shape and position of the interface. The effect of grid size and scheme on the numerical solution are crucial for convective flows with phase change [4]. In enthalpy methods (also refers as fixed grid techniques) a single set of equations is used for the entire computational domain (solid + liquid). Accurate solutions of moving boundary problems can be obtained using the enthalpy method [5]. An implicit time approximation reduces this formulation to a sequence of monotone elliptic problems which are solved by finite difference techniques [6]. A comprehensive guide for finite difference methods if phase change can be found in [7]. Eulerian-Lagrangian methods attempt to combine features of the these two methods. A Lagrangian-Eulerian approach for moving

grids was presented by [8]. Finally, a recent review of numerical techniques for solving solidification and melting phase change problems can be found in [9].

Latent heat storage using phase change materials is a common application used for the validation of a Computational Fluid Dynamics (CFD) melting and solidification model [10]. Heat is absorbed or released when the material changes from solid to liquid and vice versa. A phase change material (PCM) is a substance capable of storing and releasing large amounts of energy compared to sensible heat storage. A numerical investigation of the melting heat transfer characteristics of phase change materials in different plate heat exchanger (latent heat thermal energy storage) systems was made by [11]. Muhammad *et al.* [10] investigated the effect of liquid PCM natural convection on the latent heat storage performance of the pipe and cylinder models using a 3D numerical model with ANSYS Fluent software. Different mechanisms have been proposed to increase heat transfer in PCM, for example, using heat exchanger with fins [12]. An experimental investigation on the performance of a shell and tube heat exchanger subjected to inclination angle variation is presented in [13]. Yuan *et al.* [14] investigated the effect of fins installed at different locations on the heat transfer, and the melting characteristics of PCM in an annular with different installation angle of fins via a numerical simulation method, which is based on an enthalpy-porous medium model. Asis *et al.* (2007) [15] explored experimentally and numerically, the process of melting of a PCM in spherical geometry. Dimensional analysis of the results was performed and presented in terms of the mean Nusselt numbers and PCM melt fractions versus an appropriate combination of the Fourier, Stefan, and Grashof numbers.

Polymers have rarely been used as storage materials in latent heat storage because cyclic melting and crystallization of the material is required, and this degrades the physical properties of the material. Thermoplastics like polyethylene, polyoxymethylene and polyamides are promising PCM even as recycled material. Weingrill *et al.* (2019) [16] investigated different aging phenomena of the thermo-oxidative exposure of High-density polyethylene (HDPE) by Fourier-transform infrared spectroscopy (FTIR) and polarized light microscopy (PLM). They showed that only a small loss in the storage capacity upon thermo-oxidative exposure is detected. Therefore, HDPE proves to be a candidate material for polymeric PCM. Zauner *et al.* (2016) [17] showed that HDPE has a high phase change enthalpy and is thermally stable over more than 1000 cycles. A 3-dimensional model was implemented in ANSYS Fluent achieving excellent agreement between experiment and simulation.

Polymer recycling often requires the melting of the material before its introduction into a process chain. The recycling of polymers waste requires energy, but the energy production with conventional sources depletes the natural resources and creates environmental damages [18].

Solar thermal technology is used to collect and transform the solar energy into heat, from which 99% is used to provide warm water or space heating in residential homes, but it can also be used to provide process heat for industrial processes [19]. The temperature levels required for industrial processes heat are often higher, so concentrators and other advanced technologies are needed to increase the temperature. While concentrated radiation from solar thermal collectors have been mainly used to generate electricity and heat various fluids for energy systems, these systems have not yet been used directly for plastic recycling applications, which is the motivation of this work.

The use of renewable energy by solar concentration will be examined to perform the melting process of the polyethylene to obtain a strip of recycled material for further processing. It is important to determine the conditions in which the melting process can be carried out. The objective of this work is to understand the melting process of polymeric materials, such as high or low density polyethylene, using solar energy. Thus, the process energy is mainly supplied by radiation heat transfer, which is then transferred by heat conduction into the polymer and losses to the ambient by convection.

## 2. Problem formulation

In a general way, a Fresnel collector consists of a primary reflecting mirror that direct solar radiation to a secondary reflector (parabolic trough), which in turn, directs radiation to an absorber tube aiming to distribute it on the tube's surface homogeneously. This is shown in Fig. 1. In order to avoid convective losses in the absorber tube, it can be placed into evacuated tubes. In particular, the system of interest consists of a copper tube receiver tube located at the focal point of a Fresnell solar concentrator. The tube contains a polymeric material, like HDPE or LDPE. Since the main purpose of this study is to determine the conditions (solar radiation and convective losses) in which the melting process of the polymeric

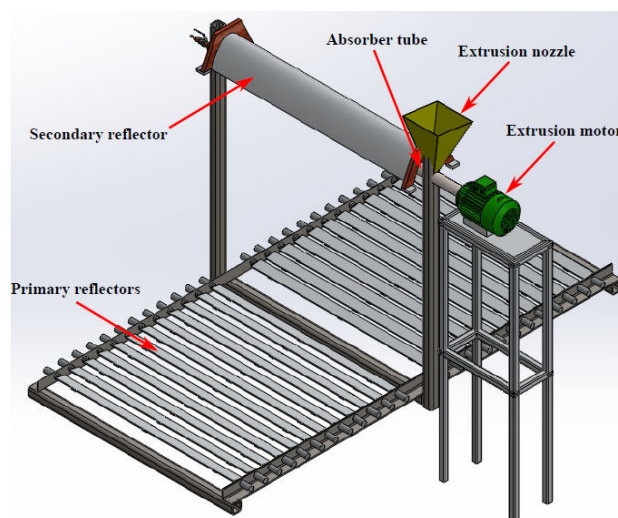


FIGURE 1. Scheme of the Fresnell solar concentrator.

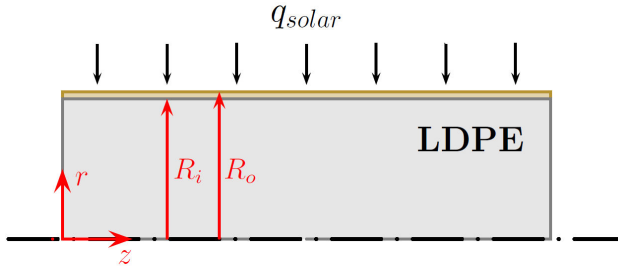


FIGURE 2. Diagram of the cylindrical rod considered in this study.

polymeric material can be carried out, no input flow throughout the tube is considered. Even though, the proposed design includes an extrusion system (nozzle and motor) that would drive the molten material which otherwise would not flow given its high viscosity. Since the main purpose of this study is to determine the conditions (solar radiation and convective losses) in which the melting process of the polymeric material can be carried out, no input flow throughout the tube is considered.

In the most simple case, it can be considered a cylindrical rod of LDPE, as shown in Fig. 2. It is assumed that the thermal conductivity of the tube wall is much higher than the thermal conductivity of the PCM and the ratio of the outer to the inner diameters is approximately one ( $R_o/R_i \approx 1$ ), which allows neglecting the thickness of the tube wall. Additionally, the length of the rod is much bigger than its diameter, and thus changes in the axial direction can be disregarded. Under these assumptions the problem can be reduced to two dimensions ( $r, \theta$ ), or even to one dimension ( $r$ ), if the incident radiation is homogeneously distributed on the cylinder surface.

### 3. Mathematical formulation

Heat transfer during the plastic melting process can be described by a couple of equations, one for the solid and the other for the liquid. In one dimension these equations read as follows:

$$\frac{1}{r} \frac{\partial}{\partial r} \left( k_s r \frac{\partial T_s}{\partial r} \right) = \rho_s c_s \frac{\partial T_s}{\partial t}, \quad 0 \leq r < R(t), \quad (1)$$

$$\frac{1}{r} \frac{\partial}{\partial r} \left( k_l r \frac{\partial T_l}{\partial r} \right) = \rho_l c_l \frac{\partial T_l}{\partial t}, \quad R(t) \leq r \leq R_i, \quad (2)$$

where  $T$  is temperature;  $k$ ,  $\rho$  and  $c$  are the thermal conductivity, density and heat capacity of the materials, and the subindex  $s$  and  $l$  refer to the solid and liquid phases respectively.  $r$  is the radial coordinate and  $R(t)$  is the melting front at time  $t$ .

This case is known as Stefan's problem [1]. In the phase change interface, the temperature is continuous, and an energy balance is used

$$T_s = T_l = T_m, \quad (3)$$

$$k_s \frac{\partial T_s}{\partial r} - k_l \frac{\partial T_l}{\partial r} = \rho L \frac{\partial R(t)}{\partial t}. \quad (4)$$

TABLE I. Physical properties of LDPE (from [20]).

Solid thermal conductivity, $k_s$	0.335 W/m·K
Solid density, $\rho_s$	915 kg/m <sup>3</sup>
Solid specific heat, $c_s$	2772 J/kg·K
Melting point, $T_m$	383.15 K
Heat of fusion, $L$	$1.3 \times 10^5$ J/kg
Liquid thermal conductivity, $k_l$	0.182 W/m·K
Liquid density, $\rho_l$	810 kg/m <sup>3</sup>
Liquid specific heat, $c_l$	2604 J/kg·K

where  $L$  is the latent heat and  $T_m$  is the melting temperature.

In general, the solid and liquid densities are not the same. Usually the solid density  $\rho_s$  is greater than the liquid density  $\rho_l$  at the melting point but it can be shown that convection effects due to density differences cancel out if the solid phase density  $\rho_s$  is used in the interface energy balance equation [7]. The physical properties of LDPE can be seen in Table I.

The flow of polymeric liquids requires an understanding of the rheological behavior during processing [20]. Due to the high viscosity of the molten HDPE and the small rod diameter any natural convection flow in the melt can be neglected.

#### 3.1. The enthalpy method

The heat transfer equation can be reformulated in terms of enthalpy  $H$ , which is the sum of the sensible heat and the latent heat. In one dimension considering only heat transfer by conduction and without heat generation the enthalpy equation is

$$\frac{1}{r} \frac{\partial}{\partial r} \left( kr \frac{\partial T}{\partial r} \right) = \rho \frac{\partial H}{\partial t}. \quad (5)$$

The enthalpy is related to temperature through the equation

$$H = \begin{cases} c_s T & T < T_m, \\ c_l T + (c_s - c_l)T_m + L & T > T_m. \end{cases} \quad (6)$$

At the melting temperature  $T_m$  the enthalpy increases until the total latent heat,  $L$ , is added whereas the temperature remains constant, see [5].

Conversely, the temperature is related to enthalpy through the following equation

$$T = \begin{cases} \frac{H}{c_s} & H \leq c_s T_m, \\ T_m & c_s T_m < H \leq c_s T_m + L, \\ \frac{H - (c_s - c_l)T_m - L}{c_l} & H > c_s T_m + L. \end{cases} \quad (7)$$

In many physical problems the phase change takes place over a temperature range ( $\epsilon$ ) rather than a single value. This approach is called enthalpy linearization. In the enthalpy equation a soft region where temperature change occurs is introduced.

$$H(T) = \begin{cases} c_s T, & T \leq T_m - \epsilon, \\ c_s (T_m - \epsilon) + \left(\frac{c_s + c_l}{2} + \frac{L}{2\epsilon}\right) (T - T_m + \epsilon), & T_m - \epsilon < T < T_m + \epsilon, \\ c_l T + (c_s - c_l) T_m + L, & T_m + \epsilon \leq T. \end{cases} \quad (8)$$

With this formulation, it is possible to define another parameter that is useful for the analysis of phase change process: the liquid fraction, defined as

$$F = \begin{cases} 0, & T < T_m - \epsilon, \\ 1, & T > T_m + \epsilon, \\ \frac{T - T_m + \epsilon}{2\epsilon}, & T_m - \epsilon \leq T \leq T_m + \epsilon. \end{cases} \quad (9)$$

The dimensionless variables associated with phase change problems are the Fourier and Stefan numbers, defined as

$$\tau = \frac{\alpha t}{D^2}, \quad Ste = \frac{C_p (T_m - T_0)}{L}, \quad (10)$$

where  $D$  is the cylinder diameter,  $\alpha$  the thermal diffusivity ( $\alpha = k/C_p \rho$ ),  $t$  the time, and  $L$  the latent heat of fusion. The Fourier number  $\tau$  (also defined as  $Fo$ ) is the dimensionless time, and characterizes the transient heat transfer by conduction. Additionally, the Fourier number can be interpreted as measure of the heat conducted through the material by conduction compared to the heat stored on it. In turn, the Stefan number  $Ste$  is the ratio of the sensible heat to the latent heat of fusion.

### 3.2. Boundary conditions

The energy to carried out the melting process is considered to be obtained by solar radiation. In order to obtain the expression for the boundary condition at the surface of the rod, a heat balance is made at the external wall per unit area, which leads to

$$-k \frac{\partial T}{\partial r} = -q_{solar} + h(T - T_\infty), \quad (11)$$

where  $q_{solar}$  is the incident radiation and  $h$  the convective heat transfer coefficient, which correspond to the energy gain and losses of the material, respectively. The second boundary condition, at the axis of the cylinder, corresponds to Neumann condition,

$$\frac{\partial T}{\partial r} = 0. \quad (12)$$

## 4. Numerical Methodology

A short review of the numerical methods used to solve the phase change equations is presented in [21]. In this section the basic foundations for the development of computational code are presented. The implementation of the algorithm was done on the software Wolfram Mathematica.

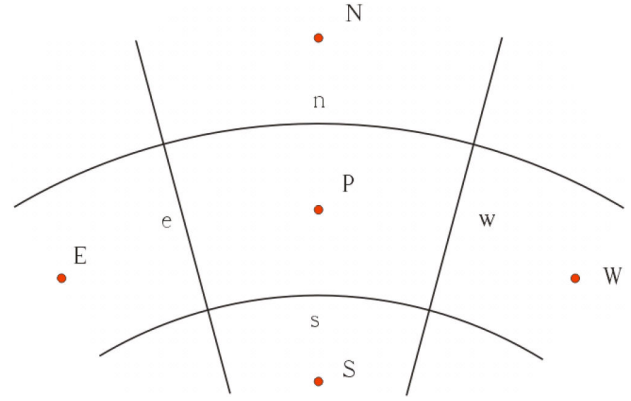


FIGURE 3. Control volume in the  $(r, \theta)$  plane of cylindrical coordinates.

### 4.1. Numerical schemes

The discrete form of the enthalpy equation is obtained with the finite volume method, integrating all terms of the phase change equation over a control volume.

The nomenclature used throughout the finite volume method is illustrated in Fig. 3. Lowercase letters are used to denote variables evaluated at the boundaries of the control volume, in the volume's contour. Uppercase letters are used to denote variables calculated at the center of the volume.

In this study, all integrals are approximated using the mid-point rule and diffusion terms are taken explicitly. The explicit finite volume representation of the Eq. (5) is

$$\rho_P (H_P - H_P^0) \frac{\delta V}{\delta t} = \left( \frac{H_N^0 - H_P^0}{\delta r} \right) k_n A_n - \left( \frac{H_P^0 - H_S^0}{\delta r} \right) k_s A_s, \quad (13)$$

where

$$A_n = r_n \delta \theta \delta z, \quad A_s = r_s \delta \theta \delta z, \quad \delta V = r_P \delta r \delta \theta \delta z. \quad (14)$$

Super index  $^0$  represents the previous time. Rearranging terms leads to the following algebraic equations

$$H_P = H_P^0 + \frac{\delta t}{\rho_P \delta V} \left( \frac{k_n A_n}{\delta r} H_N^0 + \frac{k_s A_s}{\delta r} H_S^0 - \left( \frac{k_n A_n}{\delta r} + \frac{k_s A_s}{\delta r} \right) H_P^0 \right), \quad (15)$$

The condition needed to ensure convergence is (see [5])

$$\frac{\delta t}{\delta r^2} < \frac{\rho c}{2k}. \quad (16)$$

The solution of the phase change and flow equations of molten polymers can be solved with specialized computer-aided engineering software. One tool that can be implemented is the ANSYS Fluent software that has the solidification/melting module. Instead of tracing the liquid-solid front explicitly, it uses an enthalpy formulation. COMSOL

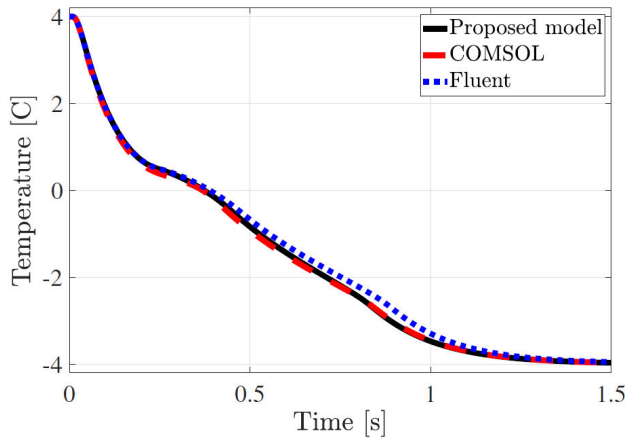


FIGURE 4. Comparison of the implemented code on Mathematica with results obtained using commercial software COMSOL and ANSYS Fluent.

Multiphysics is a finite element analysis, solver and multiphysics simulation software, in the heat transfer module we can consider phase change. Front tracking and the enthalpy formulation can be used in COMSOL.

A source code was implemented to solve the 1D phase change problem in a conductive regime. A finite volume method was implemented to discretize the governing equations. The enthalpy linearization formulation was used. In Fig. 4 results of the implemented code on Mathematica are compared with those obtained with the commercial software COMSOL and ANSYS Fluent for the benchmark case with  $c = 1 \text{ J/kg} \cdot \text{K}$ ,  $k = 1 \text{ W/m} \cdot \text{K}$ ,  $\rho = 1 \text{ kg/m}^3$  and  $L = 10 \text{ J/kg}$  which corresponds to a  $Ste = 10$ . It can be observed the good agreement between the implemented algorithm and well validated commercial software.

## 5. Results and Discussion

Once the algorithm was validated, now we explore numerically the effect of solar irradiation and heat losses by convec-

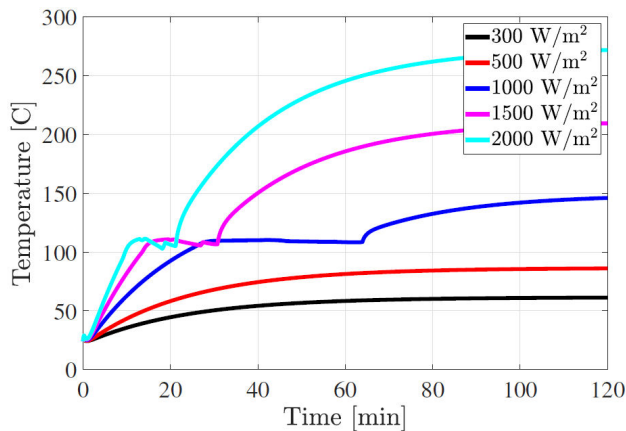


FIGURE 5. Temperature at the cylinder's centerline ( $r = 0$ ) for different radiation conditions, keeping convective losses constant.  $h = 8 \text{ W/m}^2 \cdot \text{K}$ .

tion on the phase change process. The calculations were analysed in a 3/4 inches tube containing an LDPE at an initial temperature of  $24^\circ\text{C}$  equal to ambient temperature.

Firstly, a parametric study is conducted to determine the incident radiation necessary to melt the material considering constant convective losses with a heat transfer coefficient  $h = 8 \text{ W/m}^2 \cdot \text{K}$ . In order to compare the melting process under different conditions, it can be plotted the temperature at the inner point of the material, which corresponds to the axis of the cylinder. If the temperature at this point is below the melting temperature ( $110^\circ\text{C}$ ), it implies that the whole material has been melted, and thus is able for further processing.

Figure 5 shows the temperature at the cylinder's centerline for different solar radiation. The solar radiation considered is  $q_{solar} = \{300, 500, 1000, 1500, 2000\} \text{ W/m}^2$ . Values lower than  $1200 \text{ W/m}^2$  can be easily obtained in many places worldwide without concentration, while values up to  $2000 \text{ W/m}^2$  can be easily reached, since the concentration factor is lower than 2. Higher fluxes can be captured with more sophisticated systems, as the one showed in Fig. 1. The simulation time was 2 hours, to keep time in plausible values for industrial applications. It can be observed that the complete melting of the LDPE, within the defined period, is obtained for solar irradiation higher than  $1000 \text{ W/m}^2$ . For this irradiation, full melting occurs in around 65 min. It is interesting to observe that there is no linear relation between increasing in solar radiation with decreasing in melting time. For example, double the irradiation,  $2000 \text{ W/m}^2$ , reduces the melting time to almost one third of the time it takes with  $1000 \text{ W/m}^2$ , which is ( $\sim 20 \text{ min}$ ). It is important to mention that although a greater amount of radiation could be carried out the melting process more quickly, the convective losses increase at a higher temperature, which is not considered in this case.

Figure 6 shows the evolution of the temperature in the axial line for different convective coefficients, namely  $h = \{1, 2, 4, 8, 16\} \text{ W/m}^2 \cdot \text{K}$ . This analysis allows to explore the effect of convective losses on the melting process. The higher the convective losses, the longer it takes to melt LDPE.

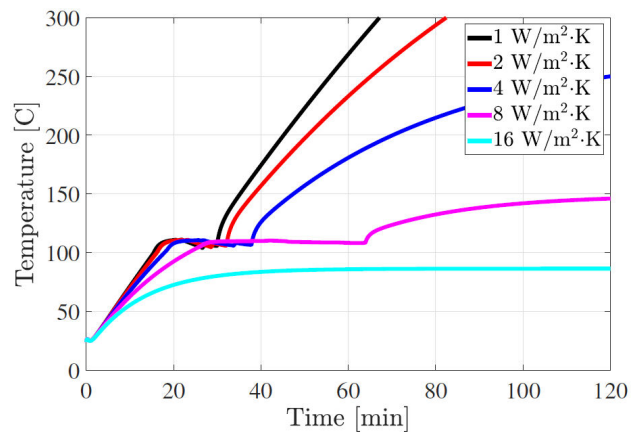


FIGURE 6. Temperature at the cylinder's centerline ( $r = 0$ ) for different convective coefficients, keeping solar radiation constant.  $q_{solar} = 1000 \text{ W/m}^2$ .

Figure 6 suggest that reducing convective heat losses reduces melting time. This can be obtained by using a vacuum tube so that all radiation received is transferred to the material (zero convective losses). Additionally, lower heat transfer coefficient improves the heat transfer process, leading to a higher operating temperature. If the losses increase to  $h = 16 \text{ W/m}^2\cdot\text{K}$ , it is not possible to reach the melting temperature in the considered operating time.

### 6. Conclusions

In this work, a preliminary study of the melting process of a polymeric material like LDPE have been investigated numerically. For this purpose a numerical code has been implemented in Wolfram Mathematica. This code was validated against commercial software COMSOL Multiphysics and ANSYS Fluent. The developed code is in good agreement with commercial software results. The effect of solar irradiation and heat losses by convection on the phase change process has been explored. Computational modeling allows to estimate the operating conditions under which the complete melting of the LDPE can be obtained. This study provides some insights that will help in the design of a prototype that guarantees the successful recycling process. Future work include the fabrication and instrumentation of the design presented in Fig. 1. This will allow the validation of this simple model. Additionally, experimental results will provide valuable information that might be used to improve existing models and implement new ones. Among the phenomena that require to be included in the model are the inhomogeneity in surface heating and fluid flow, that in this work are disregarded but may induce instabilities in the flow and thus will affect the melting process.

#### List of Symbols

Greek letters	
$\rho$	Density (kg/m <sup>3</sup> )
$\tau$	Fourier number
$\delta t$	time step

$\delta x$	Cell length
$\theta$	Angular coordinate
$\epsilon$	Temperature range
Nomenclature	
$T$	Temperature (K)
$k$	Thermal conductivity (W/m·K)
$H$	Enthalpy (J)
$F$	Liquid fraction
$A$	Area
$R$	Radius (m)
$c$	Heat capacity (J/kg·K)
$L$	Heat of fusion (J/kg)
$Ste$	Stefan number
Subscripts	
$s$	Solid
$l$	Liquid
$o$	outer
$m$	melting
$N$	North
$S$	South
$E$	East
$W$	West
$P$	Center

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